

Crossover properties of a one-dimensional reaction-diffusion process with a transport current

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Abstract. One-dimensional models of particles subjected to a coagulation-diffusion process are important in understanding non-equilibrium dynamics, and fluctuation-dissipation relation. We consider in this paper transport properties in finite and semi-infinite one-dimensional chains. A set of particles freely hop between nearest-neighbor sites, with the additional condition that, when two particles meet, they merge instantaneously into one particle. By imposing a localized source of particle-current at the origin and a non-symmetric hopping rate between the left and right directions (particle drift), we obtain exact expressions for the particle-density, current and coagulation rate in the continuum limit as function of time and position. These results are derived from the empty-interval-particle method, where the probability of finding an empty interval between two given sites is considered as the fundamental function for evaluating transport quantities. Closed equations are obtained for this quantity, depending on initial and boundary conditions, and a crossover behavior is studied between an algebraic and exponential decay of the particle density.

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1. Introduction

Non-equilibrium phenomena in strongly interacting many-body systems often provide complex interactions between fluctuation and dissipation processes, which constitutes an important field of ongoing research [1, 2]. Fluctuations in one dimension are so large that mean field methods are irrelevant, instead exact results are necessary but not always possible. One simple model possessing strong fluctuations and critical behavior is represented by the diffusion-coagulation process of indistinguishable particles on a discrete chain where each site of elementary size a contains at most one particle. The dynamics is defined by particles A that can hop between neighboring sites $A + \emptyset \rightarrow \emptyset + A$ or $\emptyset + A \rightarrow A + \emptyset$ with a rate Γ and eventually coagulate $A + A \rightarrow A$ when two particles meet on the same site with probability unity. This model is exactly solvable and the density of particles in the continuum limit, when the product $\Gamma a^2 =: \mathcal{D}$ (diffusion coefficient) is kept constant when a goes to zero, is known to decrease with time like $t^{-1/2}$ (see [3] for a detailed review) in the long-time limit (scaling regime), instead of t^{-1} in the mean-field approximation, implying strong fluctuation effects. Experimentally, such effects have been observed experimentally, in the kinetics of quasi-particles called excitons on long chains of polymers TMMC=(CH₃)₄N(MnCl₃) [4], and in other types of polymers [5, 6] almost one dimensional. Interesting quantities such as two-point correlation functions and response functions [7, 8, 9] can be explicitly evaluated in the continuum limit, invalidating the direct applicability of the fluctuation-dissipation theorem. Introducing external sources is a usual tool to probe the dynamics and influence of the different time scales in the different transient regimes. Influence of sources was studied in the case of uniform particle deposition with a given constant rate [10, 11, 12] or charge deposition [13] on random chosen sites in one dimensional chains, or even in membranes [14]. In the coagulation-diffusion model, the equation of diffusion for the probability of an empty interval of size x is modified by a source term proportional to the size x . This equation admits solutions in terms of the Airy function, with eigenvalues proportional to the zeros of this function. It shows interestingly that no first-order rate equation can be written explicitly, except in the asymptotic regime near the stationary state. Relaxation behavior was also studied in the one-dimensional charge aggregation model [15, 13], where particles can coagulate by addition of their charge, and time power law or stretched exponential dependence was found by studying how an excitation charge (or pair of opposite charges) is dissipated into the system by studying the Green function behavior in the long-time regime.

Here in this paper we consider the dynamics of a coagulation-diffusion process on a finite and semi-infinite chain with a source of particles at the origin and eventually an asymmetric hopping rate. The aim is to probe the different time scale regimes and steady states, by varying the input current and particle drift, or biased diffusion. Finite size scaling was previously studied in the case of no source term, with open and periodic boundary conditions [16, 17, 18, 19]. Scaling law for the concentration $\rho_L(t) \simeq L^{-1} F_0(8\mathcal{D}t/L^2)$ in a finite chain of size L and diffusion constant \mathcal{D} was derived and expressed in particular with Jacobi theta functions, reflecting the Gaussian or diffusive

character of the Green function in the finite case. In the following, we consider the possibility of having different crossover regimes in the case of an input current at the origin, which introduces another time scale in the system, or coherent length, after the characteristic time of diffusion through the system $L^2/(8\mathcal{D})$ is reached, and from an initial state where every site is occupied by a particle. Such model was studied with a particle input at the origin with open end [19], in the limit of large system size. The authors were able to extract different asymptotic regimes where the density scales like $\rho(t) \sim t^{-1/2}$ with additional corrections depending on the input rate of particles. Similarly the case with infinite input rate at both ends was also studied in a previous work [20]. The analytical treatment presented here is reminiscent of the empty-interval method conveniently used for deriving the exact two-point correlation and response functions [8, 9], in the transient and critical regimes. We can express the average density generally with a scaling function as $\rho_L(t) = L^{-1}F_0(8\mathcal{D}t/L^2, k_{in}^2 L^2)$, where k_{in} is the typical wave-length of the input current I_{in} in the continuum limit, expressed as $I_{in} = k_{in}^2 \mathcal{D}$. This scaling behavior will be exactly derived from the linear equation of motion for the probability of having no particles between two given sites (empty-interval probability). Writing the boundary conditions at both end of the chain, including the input current, symmetry relations can be found that include these boundary terms into the general Green formalism, and the continuum limit is derived in part 3, as well as the different transport quantities by using the expression of the empty-interval probability. In parts 5 and 6, we solve the local density in the semi-infinite and finite cases and study the existence of different transport regimes by identifying the crossover behaviors between the scaling regime and the finite size effect at later times, and compute the coagulation rate.

2. Empty interval probability method

We consider a finite one-dimensional chain of N sites filled with particles (\bullet) or empty sites (\circ). Particles can diffuse inside the chain with asymmetric rate $\alpha\Gamma$ to the right, with $\alpha \geq 1$, and with rate Γ to the left. They can also merge (coagulation) on the same site with probability unity. A flux of new particles is introduced from the left hand side of the chain with rate $\beta\Gamma$.

2.1. Definition of the model and equations of motion in the discrete case

A convenient way to describe in general coagulation-diffusion processes is to introduce the empty-interval probability $E_{n_1, n_2}(t) = \Pr(n_1 \boxed{\text{d}} n_2)$ for $0 \leq n_1 \leq n_2 \leq N$, $d = n_2 - n_1$, which physically represents the probability to have only empty sites at least inside the interval $[n_1, n_2]$ of size d . The boundary condition of zero size interval is given by $E_{n_1, n_1}(t) = 1$, which is the probability to find no particle. Inside the chain, after an elementary time step Δt , we can write the following discrete equation of evolution

$$\frac{E_{n_1, n_2}(t + \Delta t) - E_{n_1, n_2}(t)}{\Delta t} = \Pr(\curvearrowright n_1 \boxed{\bullet \text{d} - 1} n_2) + \Pr(n_1 \boxed{\text{d} - 1 \bullet} n_2 \curvearrowleft)$$

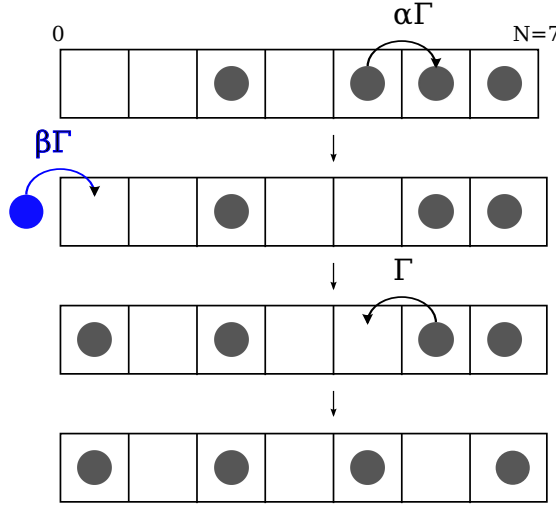


Figure 1. Example of a chain of length $N = 7$ filled partially with particles (disks). One time processes occur when particles diffuse to the left or right with rate Γ and $\alpha\Gamma$ respectively. Particles can exit the last site on the right with rate $\alpha\Gamma$ and enter from the left with a different rate $\beta\Gamma$ (input current).

$$-\Pr(\bullet \curvearrowright n_1 \boxed{\text{d}} n_2) - \Pr(n_1 \boxed{\text{d}} n_2 \curvearrowleft \bullet). \quad (1)$$

The different transition rates on the right hand side can be computed using conservative relations between probabilities, for example for the first term we can write

$$\begin{aligned} \Pr(\curvearrowleft n_1 \boxed{\bullet \text{ d-1}} n_2) &= \Gamma \times \Pr(n_1 \boxed{\bullet \text{ d-1}} n_2), \\ \Pr(n_1 \boxed{\bullet \text{ d-1}} n_2) + \Pr(n_1 \boxed{\circ \text{ d-1}} n_2) &= \Pr(n_1 + 1 \boxed{\text{d-1}} n_2), \\ \Pr(n_1 \boxed{\bullet \text{ d-1}} n_2) &= E_{n_1+1, n_2} - E_{n_1, n_2}, \end{aligned} \quad (2)$$

and we obtain, for the dynamics inside the bulk, the following dynamical equation

$$\begin{aligned} \frac{E_{n_1, n_2}(t + \Delta t) - E_{n_1, n_2}(t)}{\Delta t} &= \Gamma \left[E_{n_1-1, n_2}(t) + E_{n_1+1, n_2}(t) + E_{n_1, n_2-1}(t) + E_{n_1, n_2+1}(t) \right. \\ &\quad \left. - 4E_{n_1, n_2}(t) \right] + (\alpha - 1)\Gamma \left[E_{n_1, n_2-1}(t) + E_{n_1-1, n_2}(t) - 2E_{n_1, n_2}(t) \right]. \end{aligned} \quad (3)$$

The last term in brackets corresponds to the drift contribution $(\alpha - 1) \neq 0$ which vanishes when the dynamics is symmetric. The first term in brackets is the classic diffusion process inside the bulk.

2.2. Boundary conditions

Boundary conditions at locations $n_1 = 0$ and $n_2 = N$ are found by writing the equations of motions at these points. New particles can enter the left hand side of the chain with rate $\beta\Gamma$ and

diffuse through the system with rates Γ or $\alpha\Gamma$ before eventually exit the chain on the right with probability $\alpha\Gamma$. In the limit $\Delta t \rightarrow 0$, we have

$$\frac{\partial E_{0,n_2}(t)}{\partial t} = \Pr(0 \boxed{\text{d-1 } \bullet} n_2 \curvearrowright) - \Pr(0 \boxed{\text{d}} n_2 \curvearrowright \bullet) - \Pr(\bullet \curvearrowright 0 \boxed{\text{d}} n_2).$$

The last probability is equal to $\Pr(\bullet \curvearrowright 0 \boxed{\text{d}} n_2) = \beta\Gamma \times \Pr(0 \boxed{\text{d}} n_2) = \beta\Gamma E_{0,n_2}(t)$ and we obtain

$$\frac{\partial E_{0,n_2}(t)}{\partial t} = \Gamma \left[E_{0,n_2-1}(t) + E_{0,n_2+1}(t) - (1 + \alpha + \beta) E_{0,n_2}(t) \right]. \quad (4)$$

Comparing Eq. (4) with Eq. (3), we can formally extend the first index n_1 to negative values, by imposing the relation $\alpha E_{-1,n_2}(t) + E_{1,n_2}(t) = (1 + \alpha - \beta) E_{0,n_2}(t)$ and which gives a condition of continuity between probabilities with negative index $n_1 = -1$ and positive $n_1 = 1$. By deriving successively this relation with respect with time t , we obtain a more general symmetry identity

$$\alpha^{n_1} E_{-n_1,n_2}(t) + E_{n_1,n_2}(t) = \mathcal{A}(n_1) E_{0,n_2}(t), \quad (5)$$

where $\mathcal{A}(n)$ satisfies the discrete equation $\mathcal{A}(n+1) + \alpha\mathcal{A}(n-1) = \mathcal{A}(1)\mathcal{A}(n)$, with $\mathcal{A}(1) = (1 + \alpha - \beta)$ and $\mathcal{A}(0) = 2$. The unique solution of this equation is given by

$$\mathcal{A}(n) = (2\alpha)^n (r_1^{-n} + r_2^{-n}), \quad (6)$$

with $r_1 r_2 = 4\alpha$ and $r_1 + r_2 = 2(1 + \alpha - \beta)$. On the right (open) boundary of the chain, we have instead

$$\frac{\partial E_{n_1,N}(t)}{\partial t} = \Pr(\curvearrowleft n_1 \boxed{\bullet \text{d-1}} N) + \Pr(n_1 \boxed{\text{d-1 } \bullet} N \curvearrowright) - \Pr(\bullet \curvearrowleft n_1 \boxed{\text{d}} N),$$

or, after some algebra

$$\frac{\partial E_{n_1,N}(t)}{\partial t} = \Gamma \left[\alpha E_{n_1-1,N}(t) - E_{n_1,N}(t) + E_{n_1,N-1}(t) - E_{n_1,N}(t) - E_{n_1,N}(t) + E_{n_1-1,N}(t) \right]. \quad (7)$$

Comparing Eq. (7) with Eq. (3), we obtain formally the condition $E_{n_1,N}(t) = E_{n_1,N+1}(t)$. Taking the time derivative of this identity, the next relation yields to $E_{n_1,N+2}(t) = (1 - \alpha) E_{n_1,N}(t) + \alpha E_{n_1,N-1}(t)$. More generally, it is straightforward to prove recursively by successive derivations that

$$E_{n_1,N+k}(t) = \sum_{l=0}^{k-1} \mathcal{B}(k,l) E_{n_1,N-l}(t), \quad (8)$$

with the coefficients \mathcal{B} satisfying the discrete recursive equations

$$\begin{aligned}\mathcal{B}(k+1, 0) &= \mathcal{B}(k, 0) + \mathcal{B}(k, 1) - \alpha\mathcal{B}(k-1, 0), \\ \mathcal{B}(k+1, l) &= \mathcal{B}(k, l+1) + \alpha\mathcal{B}(k, l-1) - \alpha\mathcal{B}(k-1, l), \text{ for } 1 \leq l \leq k-2, \\ \mathcal{B}(k+1, k-1) &= \alpha\mathcal{B}(k, k-2), \text{ and } \mathcal{B}(k+1, k) = \alpha\mathcal{B}(k, k-1).\end{aligned}\quad (9)$$

By inspection, we found the boundary conditions $\mathcal{B}(1, 0) = 1$, $\mathcal{B}(k \geq 2, 0) = 1 - \alpha$, and generally $\mathcal{B}(k, l) = (1 - \alpha)\alpha^l$ for other values of l , except for the last term $\mathcal{B}(k+1, k) = \alpha^k$.

3. Continuum limit and symmetry equations

In this section we consider the continuum limit of Eq. (3), including the different boundary conditions previously obtained. If a is the elementary lattice step, we introduce coordinates $x_1 = n_1 a$ and $x_2 = n_2 a$, while $L = Na$ is finite when $a \rightarrow 0$. In this case $E_{n_1, n_2}(t) \rightarrow E(x_1, x_2; t)$ and Eq. (3) becomes the equation of diffusion

$$\frac{\partial E(x_1, x_2; t)}{\partial t} = \mathcal{D} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) E(x_1, x_2; t) - v \left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) E(x_1, x_2; t), \quad (10)$$

where $\mathcal{D} = \Gamma a^2$ is the diffusion coefficient in the limit $a \rightarrow 0$, and $v = 2k_b \mathcal{D}$ is the drift velocity, k_b being the characteristic momentum coming from the scaling $\alpha = 1 + 2k_b a$ (see Table 1). Eq. (10) is solved using a double Fourier transform $E(x_1, x_2; t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dk_1 dk_2}{4\pi^2} \exp(ik_1 x_1 + ik_2 x_2) \tilde{E}(k_1, k_2; t)$, and the evolution of the empty-interval probability as function of initial conditions is given by

$$\begin{aligned}E(x_1, x_2; t) &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dx'_1 dx'_2}{4\pi \mathcal{D} t} \exp \left[-\frac{1}{4\mathcal{D} t} (x_1 - x'_1 - vt)^2 - \frac{1}{4\mathcal{D} t} (x_2 - x'_2 - vt)^2 \right] E(x'_1, x'_2; 0) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'_1 dx'_2 \mathcal{W}_{l_0}(x_1 - x'_1) \mathcal{W}_{l_0}(x_2 - x'_2) E(x'_1, x'_2; 0), \\ \mathcal{W}_{l_0}(x) &:= \sqrt{\frac{2}{\pi l_0^2}} \exp \left\{ -2(x - vt)^2 / l_0^2 \right\}.\end{aligned}\quad (11)$$

The integrals over the real axis in the previous expression are unrestricted. We also have introduced the classical diffusion length $l_0 := \sqrt{8\mathcal{D}t}$, which acts as the typical scaling length in the problem \ddagger . The different physical parameters and their continuous versions are given in Table

\ddagger In the context of the coagulation-diffusion problem on an infinite chain and without drift, the probability is invariant by translation and $E(x_1, x_2; t)$ can be written as $E(x_2 - x_1; t)$. In Eq. (11), the change of variable $y_1 = x'_2 - x'_1$ and $y_2 = x'_2 - x_2$, such that $(x_1 - x'_1)^2 + (x_2 - x'_2)^2 = (x_2 - x_1 - x'_2 + x'_1)^2 + 2(x_2 - x'_2)(x_1 - x'_1) = (x_2 - x_1 - y_1)^2 + 2y_2(y_2 - y_1 + x_2 - x_1)$, and the Gaussian integration on y_2 lead to the one-interval solution $E(x_2 - x_1; t) = \int_{-\infty}^{\infty} \frac{dy_1}{\sqrt{\pi} l_0} \exp \left[-\frac{1}{l_0^2} (x_2 - x_1 - y_1)^2 \right] E(y_1; 0)$.

1. We now treat the boundary conditions in the continuous limit. On the left hand side of the chain, around the origin, the symmetry Eq. (5) has a continuous solution given by

$$e^{2k_b x_1} E(-x_1, x_2; t) + E(x_1, x_2; t) = \mathcal{A}(x_1) E(0, x_2; t), \quad (12)$$

where $\mathcal{A}(n) \rightarrow \mathcal{A}(x = nL)$ satisfies the differential equation

$$\mathcal{A}''(x) - 2k_b \mathcal{A}'(x) + k_{in}^2 \mathcal{A}(x) = 0, \quad (13)$$

with initial conditions $\mathcal{A}(0) = 2$ and $\mathcal{A}'(0) = 2k_b$. This equation is deduced from the discrete recursion for $\mathcal{A}(n)$, and from the natural scaling $\beta = a^2 k_{in}^2$ where k_{in} is the input momentum. Indeed, the input current is given by $I_{in} = \Gamma\beta$ which has the finite value $I_{in} = \mathcal{D}k_{in}^2$ by replacing β with the corresponding scaling. In particular, the continuous limit of the discrete Eq. (5) $\alpha E_{-1,n_2}(t) + E_{1,n_2}(t) = (1 + \alpha - \beta)E_{0,n_2}(t)$ gives $\partial_{x_1}^2 E(0, x_2; t) - 2k_b \partial_{x_1} E(0, x_2; t) = -k_{in}^2 E(0, x_2; t)$ for intervals incorporating the origin. We may then identify k_{in} with the inverse of a coherent length inside the chain, in the sense that empty intervals are suppressed by large input currents. Then the solution for Eq. (6) in the continuum limit, or Eq. (13), is given by $\mathcal{A}(x) = 2 \exp(k_b x) \cosh(x \sqrt{k_b^2 - k_{in}^2})$. The cosh function is transformed into a cosine function when $k_{in} > k_b$, or $\mathcal{A}(x) = 2 \exp(k_b x) \cos(x \sqrt{k_{in}^2 - k_b^2})$. We also have a symmetry equation by exchanging the position variables of the interval [13, 21]

$$E(x_1, x_2; t) = 2 - E(x_2, x_1; t), \quad (14)$$

which holds even in presence of a drift term v . The continuum version of the other boundary condition Eq. (8) can be found by noticing that the sum of terms proportional to $(1 - \alpha) = -2k_b a$ becomes an integral, and coefficients α^l with $l \geq 0$, in Eq. (8), have a finite limit $\mathcal{B}(x) := \exp(2k_b x)$ with $x = la$. Then we obtain the symmetry equation

$$E(x_1, L + x_2; t) = \exp(2k_b x_2) E(x_1, L - x_2; t) - 2k_b \int_0^{x_2} dy \exp(2k_b y) E(x_1, L - y; t). \quad (15)$$

It is useful to define the new function $\hat{E}(x_1, x_2; t) := \exp[-k_b(x_1 + x_2)] E(x_1, x_2; t)$, in order to simplify the different symmetry relations given by the set of three equations

$$\begin{aligned} \hat{E}(x_1, x_2; t) + \hat{E}(-x_1, x_2; t) &= \hat{\mathcal{A}}(x_1) \hat{E}(0, x_2; t), \quad \hat{\mathcal{A}}(x_1) := 2 \cosh\left(x_1 \sqrt{k_b^2 - k_{in}^2}\right), \quad (a) \\ \hat{E}(x_1, x_2 + L; t) &= \hat{E}(x_1, L - x_2; t) - 2k_b \int_0^{x_2} dy \exp[2k_b(y - x_2)] \hat{E}(x_1, L - y; t), \quad (b) \\ \hat{E}(x_1, x_2; t) + \hat{E}(x_2, x_1; t) &= 2 \exp[-k_b(x_1 + x_2)]. \quad (c) \end{aligned} \quad (16)$$

In the following, we will consider two cases. The semi-infinite system with $L = \infty$, where symmetries Eq. (16) reduce to (a) and (c), and the finite system with no drift term $k_b = 0$. In both cases, the interval probability function can be computed explicitly. In the next section, we define the important transport quantities in the continuum limit that are used in the next part of the paper, such as the particle density or current as function of space and time.

3.1. Transport quantities

We define in this part the average density and current inside the chain. The different notations throughout the text for defining the different physical quantities can be found in Table 1. The local density is noted $\rho_n(t)$ (or $\rho(x; t)$ in the continuum limit), and is defined by $\Pr(n \blacksquare n+1)/a$ which is equal to $(1 - E_{n,n+1}(t))/a \simeq -\partial_2 E(x, x; t)$. Short notation ∂_i , with $i = 1, 2$, is meant for partial derivation with respect to component x_i . Similarly, we can write $\rho_n(t) = \Pr(n-1 \bullet n)/a \simeq \partial_1 E(x, x; t)$, and therefore, by symmetry,

$$\rho(x; t) = \frac{1}{2}(\partial_1 - \partial_2)E(x, x; t). \quad (17)$$

We also define a local current $I_n(t)$ (or $I(x; t)$ in the continuum limit) as the probability rate for a particle (with discrete velocities $a\Gamma$ and $\alpha a\Gamma$) to move to the right of a given location minus the probability for another particle to move to the left of the same point

$$I_n(t) := \Pr(n-1 \bullet n \curvearrowright) - \Pr(\curvearrowleft n \blacksquare n+1). \quad (18)$$

This can be written as function of the interval probabilities

$$\begin{aligned} I_n(t) &= \Gamma [\alpha \Pr(n-1 \bullet n) - \Pr(n \blacksquare n+1)] \\ &= \Gamma(\alpha - 1) + \Gamma [E_{n,n+1}(t) - \alpha E_{n-1,n}(t)] \\ &\Rightarrow I(x; t) = \frac{\mathcal{D}}{2} [4k_b \partial_1 E(x, x; t) + (\partial_2^2 - \partial_1^2)E(x, x; t)] \\ &= 2k_b \mathcal{D} \partial_1 E(x, x; t) = v \rho(x; t), \end{aligned} \quad (19)$$

where we used the fact that $(\partial_1 + \partial_2)E(x, x; t) = \partial_x E(x, x; t) = 0$ deduced from the symmetry property Eq. (14) or constraint $E(x, x; t) = 1$ (and therefore $(\partial_2^2 - \partial_1^2)E(x, x; t) = (\partial_2 - \partial_1)(\partial_2 + \partial_1)E(x, x; t) = 0$). The current is simply given by the product of velocity v and the local concentration on site x . For systems with translational symmetry, $E(x_1, x_2; t) = E(x_2 - x_1; t)$, then $\partial_1 = -\partial_2$. In this case, the density is simply equal to $\rho(x; t) = -\partial_x E(x = 0; t)$ and is site-independent. The current entering the system by unit of time at the origin can be defined as the rate $\Gamma\beta$ times the probability that a particle is not present in the interval $[0, 1]$ (if a particle is already present, coagulation will occur)

$$I_{in} = \Gamma\beta \times \Pr(0 \square 1) = \Gamma\beta E_{0,1}(t) \simeq \Gamma\beta = \mathcal{D}k_{in}^2.$$

4. Semi-infinite system

When size L is infinite, symmetries Eq. (16) reduce to conditions (a) and (c). Eq. (11) can be decomposed relatively to the origin in four sectors, depending on the sign of the two coordinates

$$\begin{aligned} E(x_1, x_2; t) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx'_1 dx'_2 \widehat{\mathcal{W}}_{l_0}(x_1, x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, x'_2) \widehat{E}(x'_1, x'_2; 0) \\ &= \int_0^{\infty} \int_0^{\infty} dx'_1 dx'_2 \left\{ \widehat{\mathcal{W}}_{l_0}(x_1, x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, x'_2) \widehat{E}(x'_1, x'_2; 0) + \widehat{\mathcal{W}}_{l_0}(x_1, -x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, x'_2) \widehat{E}(-x'_1, x'_2; 0) \right. \\ &\quad \left. + \widehat{\mathcal{W}}_{l_0}(x_1, x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, -x'_2) \widehat{E}(x'_1, -x'_2; 0) + \widehat{\mathcal{W}}_{l_0}(x_1, -x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, -x'_2) \widehat{E}(-x'_1, -x'_2; 0) \right\}, \end{aligned} \quad (20)$$

with the notation $\widehat{\mathcal{W}}_{l_0}(x, y) := \mathcal{W}_{l_0}(x - y) \exp(k_b y)$. From Eq. (16), we can deduce the corresponding values in each of the sectors containing negative coordinates

$$\begin{aligned} \widehat{E}(-x'_1, x'_2) &= \widehat{\mathcal{A}}(x'_1) \widehat{E}(0, x'_2) - \widehat{E}(x'_1, x'_2), \\ \widehat{E}(x'_1, -x'_2) &= -\widehat{\mathcal{A}}(x'_2) \widehat{E}(0, x'_1) + 4e^{-k_b x'_1} \cosh(k_b x'_2) - \widehat{E}(x'_1, x'_2), \\ \widehat{E}(-x'_1, -x'_2) &= \widehat{\mathcal{A}}(x'_1) \left[2 \cosh(k_b x'_2) - \widehat{E}(0, x'_2) \right] - \widehat{\mathcal{A}}(x'_2) \left[2 \cosh(k_b x'_1) - \widehat{E}(0, x'_1) \right] \\ &\quad + 4 \sinh(k_b x'_1) \cosh(k_b x'_2) + \widehat{E}(x'_1, x'_2). \end{aligned} \quad (21)$$

The last equation can be deduced from the first two by performing symmetry operations on the first negative coordinate $-x'_1 \rightarrow +x'_1$, then on the second $-x'_2$. Another relation is also possible, by performing symmetry operations on the second coordinate $-x'_2$ first, then on $-x'_1$. A prescription is necessary in this case to obtain the correct answer: the final result will be given by taking half the sum of these two operations, yielding the third identity of Eq. (21). We then insert these expressions in Eq. (20), and rearrange the terms such that the time dependent interval probability can be written as a sum of contributions, function of initial condition $E(x_1, x_2; 0)$ with $x_1 < x_2$, in addition to those which do not depend on it. We obtain, after some algebra, and using symmetry properties in exchanging the variables of integration $x'_1 \leftrightarrow x'_2$, the following general expression

$$\begin{aligned} E(x_1, x_2; t) &= \int_0^{\infty} \int_0^{\infty} dx'_1 dx'_2 [K(x_1, x'_1) K(x_2, x'_2) - K(x_2, x'_1) K(x_1, x'_2)] E(x'_1, x'_2; 0) \theta(x'_2 - x'_1) \\ &\quad + \int_0^{\infty} \int_0^{\infty} dx'_1 dx'_2 \widehat{\mathcal{A}}(x'_1) \left[\widehat{\mathcal{W}}_{l_0}(x_1, -x'_1) K(x_2, x'_2) - \widehat{\mathcal{W}}_{l_0}(x_2, -x'_1) K(x_1, x'_2) \right] E(0, x'_2; 0) \end{aligned}$$

$$\begin{aligned}
& +1 + \int_0^\infty \int_0^\infty dx'_1 dx'_2 \left[\mathcal{W}_{l_0}(x_1 - x'_1) \mathcal{W}_{l_0}(x_2 + x'_2) - \mathcal{W}_{l_0}(x_2 - x'_1) \mathcal{W}_{l_0}(x_1 + x'_2) \right] \left[1 + e^{-2kx'_2} \right] \\
& + \left[\mathcal{W}_{l_0}(x_1 + x'_1) \mathcal{W}_{l_0}(x_2 + x'_2) - \mathcal{W}_{l_0}(x_2 + x'_1) \mathcal{W}_{l_0}(x_1 + x'_2) \right] e^{-2k_b x'_2} \\
& + \int_0^\infty \int_0^\infty dx'_1 dx'_2 \left[K(x_2, x'_1) K(x_1, x'_2) - K(x_1, x'_1) K(x_2, x'_2) \right] \theta(x'_2 - x'_1) \\
& + \int_0^\infty \int_0^\infty dx'_1 dx'_2 \widehat{\mathcal{A}}(x'_1) \left[\widehat{\mathcal{W}}_{l_0}(x_1, -x'_1) \widehat{\mathcal{W}}_{l_0}(x_2, -x'_2) - \widehat{\mathcal{W}}_{l_0}(x_2, -x'_1) \widehat{\mathcal{W}}_{l_0}(x_1, -x'_2) \right] 2 \cosh(k_b x'_2),
\end{aligned} \tag{22}$$

where $\theta(x)$ is the usual Heaviside function, equal to unity if $x > 0$, $\theta(0) = 1/2$, and zero otherwise. The kernel K is given by

$$K(x_1, x'_1) := \left[\widehat{\mathcal{W}}_{l_0}(x_1, x'_1) - \widehat{\mathcal{W}}_{l_0}(x_1, -x'_1) \right] e^{-k_b x'_1}. \tag{23}$$

Eq. (22) is consistent with the fact that E can be expressed as $1 + A(x_1, x_2)$, where A is antisymmetric: $A(x_1, x_2) = -A(x_2, x_1)$. As an application, we consider the initial conditions where the system is entirely filled with particles $E(x_1, x_2; 0) = 0$, which simplifies Eq. (22) since the first two integrals vanish. After some algebra, we find that the concentration is the sum of different contributions which can be written as

$$\begin{aligned}
\rho(x; t) = & \rho_0(x, k_b; t) + \frac{1}{4} \exp \left[(k_b - \Lambda)x - k_{in}^2 \mathcal{D}t \right] \left\{ (k_b - \Lambda) n_0(x, k_b; t) n_0(x, \Lambda; t) \right. \\
& \left. + 2\rho_0(x, k_b; t) n_0(x, \Lambda; t) - 2\rho_0(x, \Lambda; t) n_0(x, k_b; t) \right\} + \rho_1(x, k_b; t),
\end{aligned} \tag{24}$$

where we introduced the wavenumber $\Lambda := \sqrt{k_b^2 - k_{in}^2}$. Functions ρ_0 , n_0 , and ρ_1 are defined by the expressions

$$\begin{aligned}
\rho_0(x, k; t) &:= \frac{1}{\sqrt{\pi \mathcal{D}t}} \exp \left[-\frac{(x - 2k \mathcal{D}t)^2}{4 \mathcal{D}t} \right] - k e^{2kx} \operatorname{erfc} \left(\frac{x + 2k \mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) \\
n_0(x, k; t) &:= \operatorname{erfc} \left(\frac{x - 2k \mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) + e^{2kx} \operatorname{erfc} \left(\frac{x + 2k \mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right), \\
\rho_1(x, k; t) &:= \frac{1}{2\sqrt{2\pi \mathcal{D}t}} \left[\operatorname{erfc} \left(\frac{-x + 2k \mathcal{D}t}{\sqrt{2 \mathcal{D}t}} \right) - e^{4kx} \operatorname{erfc} \left(\frac{x + 2k \mathcal{D}t}{\sqrt{2 \mathcal{D}t}} \right) \right] \\
&+ \frac{k e^{4kx}}{2} \operatorname{erfc}^2 \left(\frac{x + 2k \mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) - \frac{1}{4} \partial_x \mathcal{G}_k(x, 0) \mathcal{G}_k(x, 0) \\
&- \frac{k e^{2kx}}{\sqrt{\pi \mathcal{D}t}} \int_0^\infty dy \exp \left[-\frac{(x - y - 2k \mathcal{D}t)^2}{4 \mathcal{D}t} \right] \operatorname{erfc} \left(\frac{x + y + 2k \mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right).
\end{aligned} \tag{25}$$

In the last equation, function $\mathcal{G}_k(x, y)$ is given in Appendix A by Eq. (A.2). When no source and drift are present $k_b = k_{in} = 0$, the density profile is given by the simple expression

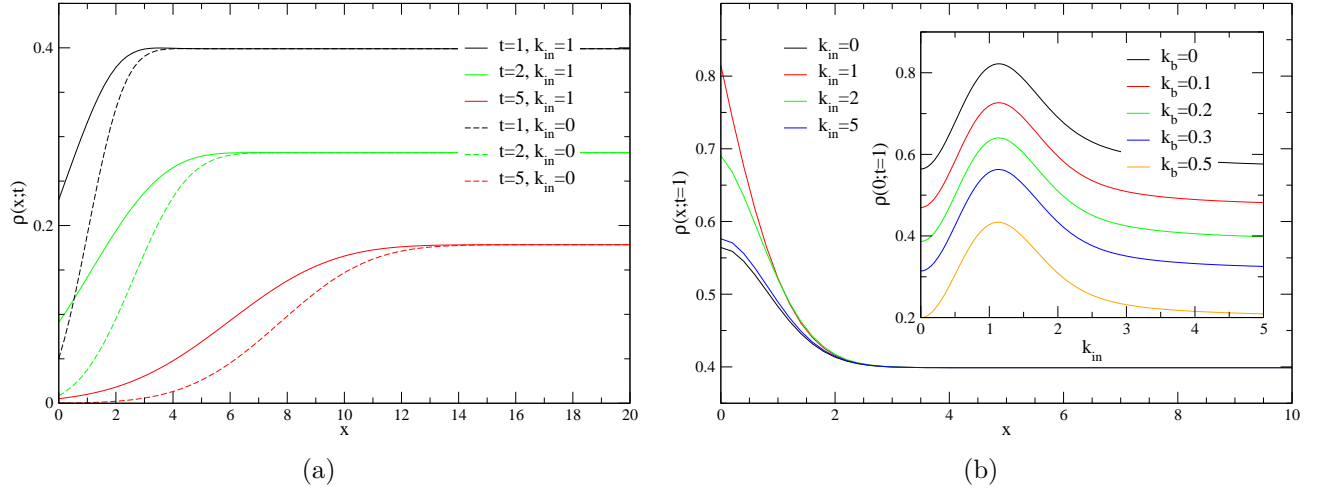


Figure 2. (a) Density profile $\rho(x;t)$ as function of time t in presence of drift $k_b = 1$ ($\mathcal{D} = 1$). Far from the origin the density is uniform and equal to $1/\sqrt{2\pi\mathcal{D}t}$. (b) Density profile in absence of drift $k_b = 0$ at time $t = 1$ ($\mathcal{D} = 1$) for several k_{in} . The density at the origin (inset) is maximum for a finite value of k_{in} , function of k_b . When k_{in} is large, the asymptotic behavior of $\rho(0;t)$ is given by the same value as $k_{in} = 0$.

$$\rho(x;t) = \frac{1}{\sqrt{\pi\mathcal{D}t}} \exp\left(-\frac{x^2}{4\mathcal{D}t}\right) \operatorname{erfc}\left(\frac{x}{2\sqrt{\mathcal{D}t}}\right) + \frac{1}{\sqrt{2\pi\mathcal{D}t}} \operatorname{erf}\left(\frac{x}{\sqrt{2\mathcal{D}t}}\right), \quad (26)$$

from which we recover the bulk density $\rho(x \gg 1;t) = (2\pi\mathcal{D}t)^{-1/2}$ far from the origin. At the origin the density is larger by a factor $\sqrt{2}$: $\rho(x=0;t) = (\pi\mathcal{D}t)^{-1/2}$, see Fig. 2(b). In Fig. 2(a) is represented the density profile for a drift momentum $k_b = 1$ (we set $\mathcal{D} = 1$), and for several values of time and input momentum k_{in} . The density (or current) at the origin grows with k_{in} as expected. In Fig. 2(b) we plotted the density profile for several input momenta k_{in} at fixed time and in absence of drift. At the origin, the concentration is given by

$$\rho(0;t) = \rho_0(0, k_b; t) + \exp(-k_{in}^2 \mathcal{D}t) [k_b - \Lambda + \rho_0(0, k_b; t) - \rho_0(0, \Lambda; t)]. \quad (27)$$

The density $\rho(0;t)$ is increasing with k_{in} up to a finite value, then decreases as the input current becomes large, see inset of Fig. 2(b). The asymptotic value is equal to the value at the origin $\rho(x \gg 1;t) = \rho(0;t)$. This feature is characteristic of coagulation-diffusion processes, since coagulation prevents the system to become overpopulated and limits the amount of particles that can be injected into the system. At the same time, diffusion tends to disperse from the origin the incoming particles, and the optimal current is given by inset of Fig. 2(b). In the next section, we focus our analysis on finite size systems.

5. Finite system with $k_b = 0$

Here we consider the case of a finite system of size L , in absence of a drift, $k_b = 0$. In Eq. (11), the integration covers the entire plane \mathbb{R}^2 inside which only the region $\mathcal{D}_0 := \{0 \leq x_1 \leq x_2 \leq L\}$ is of physical meaning. Symmetries Eq. (16) are used to fold the plane \mathbb{R}^2 into \mathcal{D}_0 , so that integrations are made only on the physical region given by initial condition $E(x_1, x_2; 0)$. Eq. (11) can be decomposed into sectors of size $L \times L$

$$E(x_1, x_2; t) = \int_0^L \int_0^L dx'_1 dx'_2 \sum_{m,n=-\infty}^{+\infty} \mathcal{W}_0(x_1 - x'_1 - mL) \mathcal{W}_0(x_2 - x'_2 - nL) \times E(x'_1 + mL, x'_2 + nL; 0). \quad (28)$$

Eq. (28) can be evaluated using the symmetries Eq. (14). For example, for $m \geq 0$, we can show recursively the following identities (after dropping the time dependence for simplification)

$$E(x_1 + mL, x_2) = \begin{cases} (-1)^p E(x_1, x_2) + \sum_{k=1}^p (-1)^{k+1} \mathcal{A}([m - 2k]L + x_1) E(0, x_2), & m = 2p \\ (-1)^p E(L - x_1, x_2) + \sum_{k=1}^p (-1)^{k+1} \mathcal{A}([m - 2k]L + x_1) E(0, x_2), & m = 2p + 1. \end{cases}$$

We can define the geometric sum $\varphi_p(x) := \sum_{k=1}^p (-1)^{k+1} \mathcal{A}(2[p - k]L + x)$, with the condition $\varphi_0(x) = 0$, which can be expressed as

$$\varphi_p(x) = \frac{\cos k_{in}[(2p - 1)L + x] - (-1)^p \cos k_{in}(L - x)}{\cos k_{in}L}. \quad (29)$$

The previous equation then becomes

$$E(x_1 + mL, x_2) = \begin{cases} (-1)^p E(x_1, x_2) + \varphi_p(x_1) E(0, x_2), & m = 2p \\ (-1)^p E(L - x_1, x_2) + \varphi_p(x_1 + L) E(0, x_2), & m = 2p + 1. \end{cases} \quad (30)$$

Also, when $m \leq 0$, we obtain after some algebra

$$E(x_1 + mL, x_2) = \begin{cases} (-1)^p E(x_1, x_2) + \varphi_p(2L - x_1) E(0, x_2), & m = -2p \\ (-1)^p E(L - x_1, x_2) + \varphi_p(L - x_1) E(0, x_2), & m = -2p + 1. \end{cases} \quad (31)$$

The two sets of conditions can be put into a more compact form such as Eq. (30) with p running from negative to positive values using, from properties of Eq. (29), the symmetry $\varphi_{-p}(x) = \varphi_p(2L - x)$, in which case Eq. (31) is equivalent to Eq. (30) by extension. Equivalently, we also have two different sets of relations for $E(x_1, x_2 + nL)$, with n either positive or negative, even or odd. However, we can use the identity $E(x_1, x_2 + nL) = 2 - E(x_2 + nL, x_1)$ and Eqs. (30)-(31) to deduce them. It is then sufficient to express $E(x_1 + 2pL, x_2 + 2qL)$ in terms of $E(x_1, x_2)$

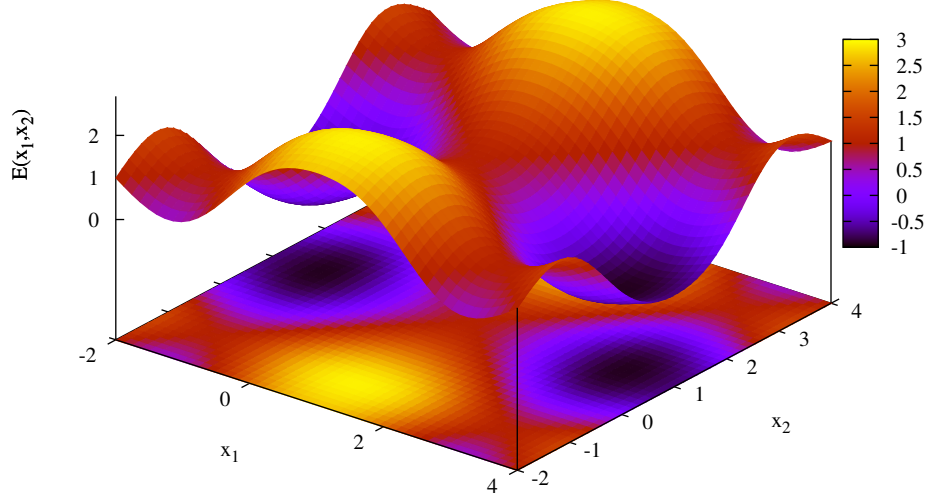


Figure 3. Example of surface $E(x_1, x_2)$ after symmetry operation for the particular initial conditions $E(x_1, x_2 > x_1; 0) = \exp[-\alpha(x_2 - x_1)^2]$, $\alpha = 10$ and $k_{in} = \pi$.

inside the physical domain \mathcal{D}_0 . This is done by applying the symmetries on the first argument $x_1 + 2pL \rightarrow x_1$, then on the second $x_2 + 2qL \rightarrow x_2$, or inversely:

$$E(x_1 + 2pL, x_2 + 2qL) = (-1)^{p+q}E(x_1, x_2) - (-1)^p\varphi_q(x_2)E(0, x_1) + (-1)^q\varphi_p(x_1)E(0, x_2) + 2(-1)^p[1 - (-1)^q] + 2\varphi_p(x_1)[1 - (-1)^q] - \varphi_p(x_1)\varphi_q(x_2) \quad (32)$$

$$E(x_1 + 2pL, x_2 + 2qL) = (-1)^{p+q}E(x_1, x_2) - (-1)^p\varphi_q(x_2)E(0, x_1) + (-1)^q\varphi_p(x_1)E(0, x_2) + 2[1 - (-1)^q] - 2\varphi_q(x_2)[1 - (-1)^p] + \varphi_p(x_1)\varphi_q(x_2). \quad (33)$$

The result depends therefore on the paths chosen in the plane to map the point $(x_1 + 2pL, x_2 + 2qL)$ onto the physical domain \mathcal{D}_0 . The correct prescription is to take half the sum of the two previous identities

$$E(x_1 + 2pL, x_2 + 2qL) = (-1)^{p+q}E(x_1, x_2) - (-1)^p\varphi_q(x_2)E(0, x_1) + (-1)^q\varphi_p(x_1)E(0, x_2) + [1 + (-1)^p][1 - (-1)^q] + \varphi_p(x_1)[1 - (-1)^q] - \varphi_q(x_2)[1 - (-1)^p]. \quad (34)$$

The resulting expression has correct symmetries and continuity. The continuity between domains of size $(L \times L)$ is satisfied using relation at the boundaries $\varphi_{p+1}(0) = \varphi_p(2L) + 2(-1)^p$. In particular, $E(x_1, x_2)$ can be formally written as before as $1 + A(x_1, x_2)$ where A is antisymmetric. In Fig. 3 is plotted the resulting surface after symmetrization for a Gaussian distribution

$E(x_1, x_2 > x_1; 0)$ with an input current, and which satisfies continuous conditions in the entire plane. The double sum in Eq. (28) can be further reduced using Eq. (34) for the odd and even integers m and n ,

$$\begin{aligned} & \int_0^L \int_0^L dx'_1 dx'_2 \sum_{m,n=-\infty}^{+\infty} \mathcal{W}_{l_0}(x_1 - x'_1 - mL) \mathcal{W}_{l_0}(x_2 - x'_2 - nL) E(x'_1 + mL, x'_2 + nL) \\ &= \int_0^L \int_0^L dx'_1 dx'_2 \sum_{p,q=-\infty}^{+\infty} \sum_{\epsilon, \epsilon'=0,1} \mathcal{W}_{l_0}(x_1 - x'_1 - \epsilon L - 2pL) \mathcal{W}_{l_0}(x_2 - x'_2 - \epsilon' L - 2qL) \\ & \times E(x'_1 + \epsilon L + 2pL, x'_2 + \epsilon' L + 2qL). \end{aligned} \quad (35)$$

We then replace $E(x'_1 + \epsilon L + 2pL, x'_2 + \epsilon' L + 2qL)$ by its value in \mathcal{D}_0 Eq. (34), and the double sum over (p, q) depends explicitly on the two Gaussian series

$$\Psi(x, y) := \sum_{p=-\infty}^{+\infty} \mathcal{W}_{l_0}(x - y - 2pL) (-1)^p, \quad \chi(x, y) := \sum_{p=-\infty}^{+\infty} \mathcal{W}_{l_0}(x - y - 2pL) \varphi_p(y), \quad (36)$$

where in particular function $\Psi(x, y)$ is anti-periodic since $\Psi(x, y + 2L) = \Psi(x + 2L, y) = -\Psi(x, y)$. For example, the first term in Eq. (34) gives

$$\sum_{p,q=-\infty}^{+\infty} \mathcal{W}_{l_0}(x_1 - x'_1 - 2pL) \mathcal{W}_{l_0}(x_2 - x'_2 - 2qL) (-1)^{p+q} E(x'_1, x'_2) = \Psi(x_1, x'_1) \Psi(x_2, x'_2) E(x'_1, x'_2).$$

The other sums over (p, q) are performed using additional functions $\Psi_s(x, y) := \Psi(x, y) - \Psi(x, -y)$ and $\chi_s(x, y) := \chi(x, y) + \chi(x, y + L)$, and symmetries $E(L + x'_1, x'_2) = E(L - x'_1, x'_2)$, $E(x'_1, L + x'_2) = E(x'_1, L - x'_2)$. After rearranging the different terms and performing change of variables in the integration over (x'_1, x'_2) , we finally obtain

$$\begin{aligned} E(x_1, x_2; t) &= 1 + G(x_1) - G(x_2) - G(x_1)F(x_2) + G(x_2)F(x_1) + F(x_1) - F(x_2) \\ & - F(x_1)F(x_2) + H(x_1, x_2) \\ & + G(x_1) \int_0^L dx'_2 \Psi_s(x_2, x'_2) E(0, x'_2; 0) - G(x_2) \int_0^L dx'_1 \Psi_s(x_1, x'_1) E(0, x'_1; 0) \\ & + \int_0^L dx'_2 \int_0^{x'_2} dx'_1 \{ \Psi_s(x_1, x'_1) \Psi_s(x_2, x'_2) - \Psi_s(x_2, x'_1) \Psi_s(x_1, x'_2) \} E(x'_1, x'_2; 0), \end{aligned} \quad (37)$$

where we defined the functions

$$F(x) := \int_0^L \Psi_s(x, x') dx', \quad G(x) := \int_0^L \chi_s(x, x') dx'. \quad (38)$$

and the contribution coming from the double integral over the ordered space variables

$$H(x_1, x_2) := 2 \int_0^L dx'_1 \Psi_s(x_1, x'_1) \int_0^{x'_1} dx'_2 \Psi_s(x_2, x'_2). \quad (39)$$

In this formula, the terms independent of the initial conditions $E(x'_1, x'_2; 0)$ in the first two lines contribute to the scaling regime, in the long time limit. It can be checked that $E(x_1, x_2) = 1 + A(x_1, x_2)$ where A is indeed antisymmetric, in particular $E(x_1, x_1) = 1$.

5.1. Expression of the current in terms of Elliptic functions

Previous functions Ψ_s and χ_s that appear in Eq. (37) can be expressed in terms of Jacobi elliptic functions θ_3 and θ_4 , after performing the sum over integers in Eq. (36). The details of the computation are given in Appendix B.

$$\begin{aligned} \Psi_s(x, y) &= \sqrt{\frac{2}{\pi l_0^2}} \left\{ e^{-\frac{2}{l_0^2}(x-y)^2} \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) - e^{-\frac{2}{l_0^2}(x+y)^2} \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x+y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) \right\}, \\ \chi_s(x, y) &= \sqrt{\frac{2}{\pi l_0^2} \frac{e^{-\frac{2}{l_0^2}(x-y)^2}}{\cos(k_{in}L)}} \left\{ \text{Re} \left[e^{ik_{in}(y-L)} \theta_3 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L} - k_{in}L, e^{-\frac{8L^2}{l_0^2}} \right) \right] \right. \\ &\quad \left. - \cos[k_{in}(y-L)] \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) \right\} + (y \rightarrow y+L). \end{aligned} \quad (40)$$

5.2. Small time behavior

For times t small compare to characteristic time $t_L := \frac{L^2}{8\mathcal{D}}$ which is the time for the particles to diffuse through the chain, the ratio L^2/l_0^2 is large, and we can replace function θ_3 and θ_4 in previous Eq. (40) by unity, since modulus $\exp(-8L^2/l_0^2)$ is exponentially small. In this case, we simply obtain

$$\Psi_s(x, y) = \sqrt{\frac{2}{\pi l_0^2}} \left\{ e^{-\frac{2}{l_0^2}(x-y)^2} - e^{-\frac{2}{l_0^2}(x+y)^2} \right\}, \quad \chi_s(x, y) = 0. \quad (41)$$

It is then straightforward to evaluate functions $F(x) = \text{erf}(\sqrt{2}x/l_0)$ and $G(x) = 0$. The local density can be generally expressed in terms of functions F , G and H

$$\rho(x; t) = (1 - F(x))G'(x) + (1 - F(x) + G(x))F'(x) + \partial_1 H(x, x). \quad (42)$$

Using $\partial_1 H(x, x) = 2 \text{erf}(2x/l_0) / \sqrt{\pi l_0^2}$, we recover Eq. (26) for a system of infinite size. Therefore, for small times the system behaves like a system of semi-infinite size without input

current. In particular, the dimensionless integrated density $\mathcal{N}_L(t) := L\rho_L(t) := \int_0^L \rho(x; t) dx$ can be expanded in terms of large parameter $L/l_0 \gg 1$

$$\mathcal{N}_L(t) \simeq \frac{2L}{\sqrt{\pi}l_0} + \frac{1}{2} - \frac{1}{\pi} + \left\{ \frac{l_0}{\sqrt{2\pi}L} - \frac{l_0^3}{4\sqrt{2\pi}L^3} \right\} \exp(-2L^2/l_0^2), \quad (43)$$

where the first term is the $1/\sqrt{t}$ law and the corrections are exponentially small in L^2/l_0^2 .

5.3. Large time expansion

In this section, we analyze the long-time limit of Eq. (40), when $l_0 \rightarrow \infty$ or $l_0 \gg L$. In this limit, it is sufficient to study the behavior of the two elliptic functions

$$\begin{aligned} \theta_3(z, \exp(-\alpha\epsilon)) &= 1 + 2 \sum_{n=1}^{\infty} \exp(-\alpha\epsilon n^2) \cos(2nz), \\ \theta_4(z, \exp(-\alpha\epsilon)) &= 1 + 2 \sum_{n=1}^{\infty} \exp(-\alpha\epsilon n^2) (-1)^n \cos(2nz), \end{aligned} \quad (44)$$

with $\alpha > 0$, z complex, and $\epsilon := L^2/l_0^2$ is the small parameter of the expansion. We can use the Dirac comb identity $\sum_{n=-\infty}^{\infty} \delta(x - n) = \sum_{n=-\infty}^{\infty} \exp(2i\pi nx)$ to rewrite $\theta_3(z, \exp(-\alpha\epsilon))$ as

$$\begin{aligned} \theta_3(z, \exp(-\alpha\epsilon)) &= \int_{-\infty}^{+\infty} dx \sum_{n=-\infty}^{\infty} \delta(x - n) \exp(-\alpha\epsilon x^2) \cos(2xz) \\ &= \int_{-\infty}^{+\infty} dx \sum_{n=-\infty}^{\infty} \exp(-\alpha\epsilon x^2 + 2i\pi nx) \cos(2xz) = \sqrt{\frac{\pi}{\alpha\epsilon}} \sum_{n=-\infty}^{\infty} \exp \left[-\frac{1}{\alpha\epsilon} \left(z + n\pi \right)^2 \right]. \end{aligned}$$

For $\theta_4(z, \exp(-\alpha\epsilon))$, the expression is identical, with instead a shift of $\pm\pi/2$ in the z argument

$$\theta_4(z, \exp(-\alpha\epsilon)) = \sqrt{\frac{\pi}{\alpha\epsilon}} \sum_{n=-\infty}^{\infty} \exp \left[-\frac{1}{\alpha\epsilon} \left(z + n\pi - \frac{\pi}{2} \right)^2 \right].$$

Setting $\alpha = 8$, $z = 4i\epsilon(x - y)/L =: 4i\epsilon(u - v)$, with $u := x/L$ and $v := y/L$, we obtain the asymptotic limit for the θ_4 function in Eq. (40)

$$\theta_4(4i\epsilon(u - v), \exp(-8\epsilon)) \simeq \sqrt{\frac{\pi}{2\epsilon}} e^{-\pi^2/(32\epsilon) + 2\epsilon(u-v)^2} \cos \left[\frac{\pi}{2}(u - v) \right]. \quad (45)$$

In the case of the θ_3 function present in Eq. (40), we take instead $z = 4i\epsilon(u - v) - k_{in}L$. The resulting θ_3 function is then complex and we obtain

$$\begin{aligned} \theta_3(4i\epsilon(u-v) - k_{in}L, \exp(-8\epsilon)) &\simeq \sqrt{\frac{\pi}{8\epsilon}} \sum_{n=-\infty}^{\infty} \exp\left[-\frac{(n\pi - k_{in}L)^2}{8\epsilon}\right] \\ &\times \exp\left[2\epsilon(u-v)^2 + i(k_{in}L - n\pi)(u-v)\right]. \end{aligned} \quad (46)$$

Most of the terms in the sum are exponentially small unless $k_{in}L$ is close to $n\pi$ with n integer. Using Eq. (45) and Eq. (46), we can evaluate directly scaling functions $\Psi_s(x, y) =: L^{-1}\tilde{\Psi}_s(u, v)$ and $\chi_s(x, y) =: L^{-1}\tilde{\chi}_s(u, v)$. In particular, we obtain asymptotically

$$\begin{aligned} \tilde{\Psi}_s(u, v) &\simeq 2e^{-\pi^2/(32\epsilon)} \sin\left(\frac{\pi u}{2}\right) \sin\left(\frac{\pi v}{2}\right), \\ \tilde{\chi}_s(u, v) &\simeq \frac{1}{\cos(k_{in}L)} \left\{ -e^{-\pi^2/(32\epsilon)} \cos\left[\frac{\pi(u-v)}{2}\right] \cos[k_{in}L(v-1)] \right. \\ &\quad \left. + \frac{1}{2} \sum_{n=-\infty}^{\infty} e^{-(n\pi - k_{in}L)^2/(8\epsilon)} \cos\left[k_{in}L(v-1) + (k_{in}L - n\pi)(u-v)\right] \right\} + (v \rightarrow v+1). \end{aligned} \quad (47)$$

The integration over v can be performed in the previous expansion, and we obtain for the functions F and G the following asymptotic results

$$\begin{aligned} F(x) &\simeq \frac{4}{\pi} e^{-\pi^2/(32\epsilon)} \sin\left(\frac{\pi x}{2L}\right) \\ G(x) &\simeq e^{-\pi^2/(32\epsilon)} \frac{\pi}{k_{in}^2 L^2 - \pi^2/4} \sin\left(\frac{\pi x}{2L}\right) + e^{-k_{in}^2 L^2/(8\epsilon)} \frac{\cos[k_{in}(x-L)]}{\cos(k_{in}L)}. \end{aligned} \quad (48)$$

In the last sum of Eq. (47), only the term $n = 0$ does not vanish after integration over variable v . Taking into account the dominant terms Eq. (48), and using the fact that H can be approximated by

$$H(x_1, x_2) \simeq \frac{16}{\pi^2} e^{-\pi^2/(16\epsilon)} \sin\left(\frac{\pi x_1}{2L}\right) \sin\left(\frac{\pi x_2}{2L}\right) = F(x_1)F(x_2), \quad (49)$$

we obtain for the expression for integrated density $\mathcal{N}_L(t)$ from expression Eq. (42)

$$\begin{aligned} \mathcal{N}_L(t) &= \frac{16k_{in}^2 L^2}{\pi(4k_{in}^2 L^2 - \pi^2)} e^{-\pi^2 t/(32t_L)} + \frac{16\pi k_{in} L \sin(k_{in}L) - 16k_{in}^2 L^2 - 4\pi^2}{\pi \cos(k_{in}L)(4k_{in}^2 L^2 - \pi^2)} e^{-(\pi^2 + 4k_{in}^2 L^2)t/(32t_L)} \\ &\quad + \frac{1 - \cos(k_{in}L)}{\cos(k_{in}L)} e^{-k_{in}^2 L^2 t/(8t_L)}. \end{aligned} \quad (50)$$

where $t_L := L^2/(8\mathcal{D})$ is the diffusion time across the system. In the absence of input current, or $k_{in} = 0$, the integrated density simply decreases like $\mathcal{N}_L(t) \simeq 4\pi^{-1} e^{-\pi^2 t/(32t_L)}$.

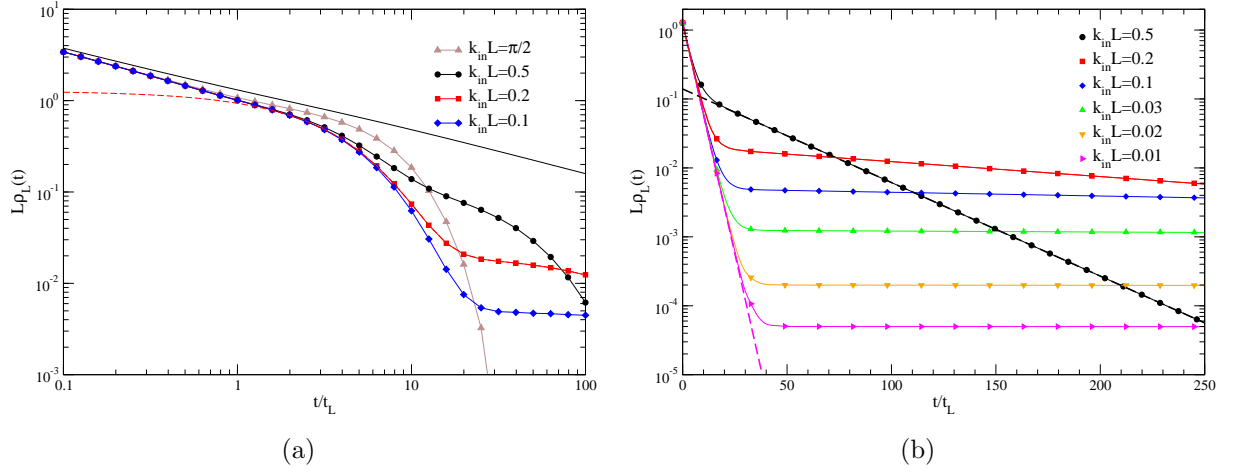


Figure 4. (a) Averaged number of particle $\mathcal{N}_L(t) = L\rho_L(t) = \int_0^L \rho(x;t) dx$ as function of time in units of $t_L = L^2/(8\mathcal{D})$ (logarithmic scale), for different values of $k_{in}L$. The chain is initially filled with particles. The curves with symbols are the numerical resolution of exact density function using expressions Eq. (40). The red dashed curve for $k_{in}L = 0.2$ is the long time behavior Eq. (50), which fits the exact solution for $t > t_L$. Black line is the density decay for the bulk regime, $L \gg 1$, given by Eq. (26). (b) Asymptotic regime $l_0 > L$ or $t > t_L$. Magenta dashed line shows the exponential decay $4\pi^{-1} \exp\{-\pi^2/(32\epsilon)\}$ in the limit $k_{in}L = 0$, and the black dashed line is the asymptotic fit, Eq. (51), for $k_{in}L = 0.5$.

In Fig. 4(a) is represented the evolution of the number of particles $\mathcal{N}_L(t)$ as function of time. For time values less than the diffusion time t_L , the number decreases like $1/\sqrt{t}$, and follows closely the result for the bulk Eq. (26). After reaching the diffusion time t_L , the number decreases exponentially like $\exp[-\pi^2 t/(32t_L)]$, independent of the input current. Then, after a crossover time $t > t_c$, the long-time regime is characterized by the experimental decay $\mathcal{N}_L \sim \exp[-k_{in}^2 L^2 t/(8t_L)]$ which depends on k_{in} . This behavior can be seen explicitly in Fig. 4(b), where the crossover is clearly visible on the averaged number $\mathcal{N}_L(t)$ as function of time (here in units of t_L) and for different values of $k_{in}L$. After a sharp decreasing behavior dominated mainly by the second term in Eq. (50), the asymptotic regime is accurately given by

$$\mathcal{N}_L \simeq \frac{1 - \cos(k_{in}L)}{\cos(k_{in}L)} \exp[-k_{in}^2 L^2 t/(8t_L)], \quad (51)$$

which is represented by the black dashed curve for $k_{in}L = 0.5$ in Fig. 4(b). The characteristic or relaxation time for this process is actually independent of the system size L , and is equal to $8t_L/(k_{in}^2 L^2) = (\mathcal{D}k_{in}^2)^{-1}$. The different curves appear to decrease more slowly as $k_{in}L$ is small. The crossover time t_c is determined by comparing the second and third terms in Eq. (50), in the limit of small $k_{in}L$ relatively to $\pi/2$:

$$t_c = \frac{32t_L}{\pi^2} \log \left[\frac{4}{\pi(1 - \cos(k_{in}L))} \right]. \quad (52)$$

For example, we obtain $t_c/t_L \simeq 13$ for $k_{in}L = 0.2$, $t_c/t_L \simeq 18$ for $k_{in}L = 0.1$, and $t_c/t_L \simeq 33$ for $k_{in}L = 0.01$, in accordance with data displayed in Fig. 4(a) and Fig. 4(b).

The final current at the end of the chain is given by the product of the probability that a particle is present in the box $[N - 1, N]$, and the rate Γ

$$I_{out}(t) = \Gamma \times \Pr(N - 1 \leq N) = \Gamma \times [1 - E_{N-1,N}(t)] \simeq -\frac{\mathcal{D}}{2} \partial_1^2 E(L, L; t).$$

We used in particular the fact that $\partial_1 E(L, L; t) = 0$ resulting from the symmetry $E(L + x_1, L) = E(L - x_1, L)$. We can then define a transfer ratio through the finite system as

$$\eta_L(t) := I_{out}(t)/I_{in} = -\frac{1}{2} k_{in}^{-2} \partial_1^2 E(L, L; t), \quad (53)$$

which evaluates the loss of particles through the system in presence of an input current. From the general Eq. (37), the current I_{out} and coefficient η_L can be evaluated, from initial conditions where the chain is entirely filled with particles $E(x_1, x_2; 0) = 0$:

$$\eta_L(t) = -\frac{1}{2} k_{in}^{-2} \left[\{1 - F(L)\} G''(L) + \{1 + G(L)\} F''(L) - F(L) F''(L) + \partial_1^2 H(L, L) \right], \quad (54)$$

Using this approximation, we obtain

$$\begin{aligned} \eta_L(t) = & \frac{2\pi}{4k_{in}^2 L^2 - \pi^2} e^{-\pi^2 t/(32t_L)} - \frac{4k_{in}^2 L^2 - \pi^2}{2\pi k_{in}^2 L^2 \cos(k_{in}L)} e^{-(\pi^2 + 4k_{in}^2 L^2)t/(32t_L)} \\ & + \frac{1}{2 \cos(k_{in}L)} e^{-k_{in}^2 L^2 t/(8t_L)}. \end{aligned} \quad (55)$$

In Fig. 5(a) is represented $\eta_L(t)$ as function of time, in units of t_L , and for several values of input current $k_{in}L$. We notice first a sharp decreasing of the output current, then a crossover towards a regime with a less pronounced variation. In particular, in the limit of small $k_{in}L \ll 1$, or very low current, $\eta_L(t)$ is close to 1/2. In this limit, we obtain the following expansion

$$\eta_L(t) \simeq \frac{1}{2} + \left[\frac{\pi}{2k_{in}^2 L^2} + \frac{\pi}{4} - \frac{4}{\pi} - \frac{\pi t}{16t_L} \right] e^{-\pi^2 t/(32t_L)}, \quad (56)$$

for which the value 1/2 is reached during an interval of time $t_L < t$. Oppositely, Fig. 5(b) represents the ratio $\eta_L(t)$ as function of $k_{in}L$ for different time values. As the size L of the system increases, the ratio goes to zero monotonically as expected. Finally, we can use expressions Eq. (50)

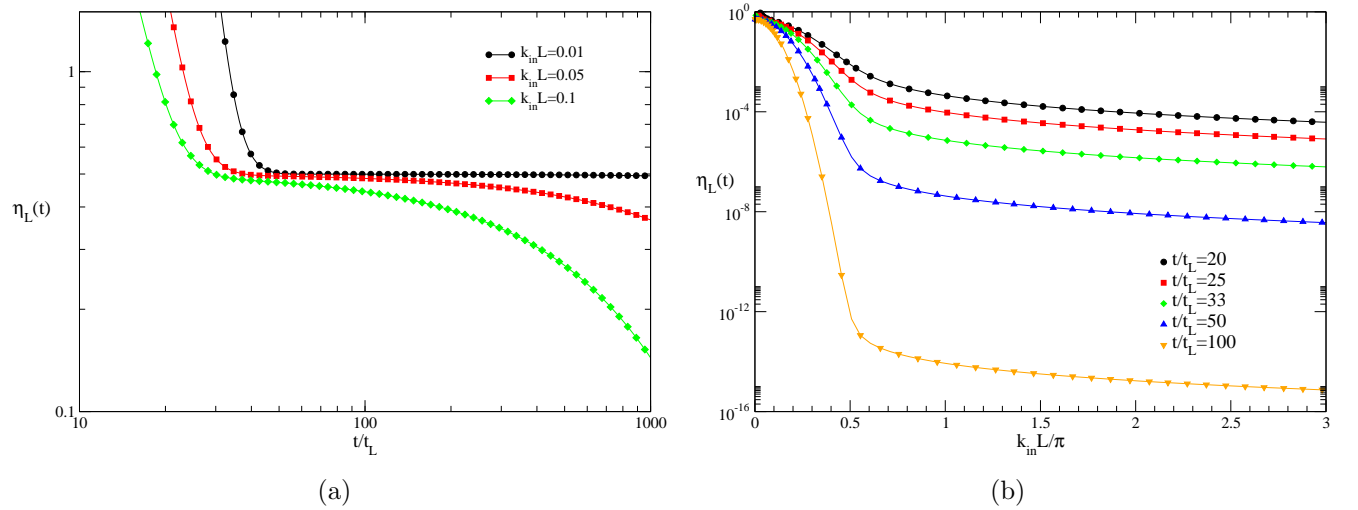


Figure 5. (a) Current ratio $\eta_L(t) = I_{out}(t)/I_{in}$ as function of time t , in units of $t_L = L^2/(8\mathcal{D})$, for different values of parameter $k_{in}L$ in the asymptotic regime $t \gg t_L$, or when $\epsilon = t_L/t$ is small. The current ratio appears to stabilize around 1/2 when $k_{in}L$ is small, before decreasing at later times. (b) Current ratio as function of $k_{in}L$ for different time values.

and Eq. (55) to compute the rate of coagulation $R_c > 0$ in the system as function of time, by considering the terms contributing to the loss and gain of particles

$$\frac{d\mathcal{N}_L(t)}{dt} = I_{in} - I_{out} - R_c = I_{in} [1 - \eta_L(t)] - R_c. \quad (57)$$

In the long time limit, and for small input current $k_{in}L \ll 1$, we obtain the following expansion

$$R_c \simeq \frac{1}{2}I_{in} + \frac{\pi}{16t_L}e^{-\pi^2 t/(32t_L)} + 8I_{in}e^{-\pi^2 t/(32t_L)} \left[\frac{3}{2\pi} - \frac{1}{2} + \frac{\pi}{32} - \frac{\pi t}{128t_L} \right], \quad (58)$$

which shows that half of the input particles coagulate, plus corrective terms which are exponentially small, the last term being negative in this limit. These corrections arise from the finiteness of the system and depends on the time for the input particles to reach the opposite border.

6. Conclusion

In this paper, we presented an application of the empty interval method to the transport properties in a reaction-diffusion process, with semi-infinite and finite geometries. This method is well adapted in computing density and current quantities using only a two-space variable interval probability which satisfies a classical linear equation of diffusion, which measures specifically the probability of having an empty space between two sites. The essential point is to treat the

boundary conditions, since there no possibility to use translation invariance, by incorporating the boundary terms into the symmetries of the probability function. This can be done by extending the problem to the real axis, and by introducing a mirror-image method that takes exactly into account the different symmetries relating negative and positive interval distances. The effect of a current at the origin, which probes the dynamics for a finite or semi-infinite system, is to introduce different time scales, one short time scaling regime, where the density scales like $t^{-1/2}$, and an exponential decay, once the time reaches the typical diffusion time scale through the chain, whose relaxation constant depends on the current value. We were also able to compute the coagulation rate in the asymptotic regime by studying the balance between the different reaction rates. The semi-infinite chain with asymmetry diffusion rate shows the existence of an optimal current which maximizes the particle density near the origin.

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We would like to acknowledge M. Henkel and J. Richert for informal discussions on this topic.

Table 1. Notations for the physical quantities

a	lattice step	L	system size
Γ	diffusion rate to the left	$\mathcal{D} = \Gamma a^2$	diffusion constant
$\alpha\Gamma$	diffusion rate to the right	$\beta\Gamma$	input rate of particles
$\alpha = 1 + 2k_b a$	scaling limit for α	$k_{in} = \sqrt{\beta}/a$	input momentum
$v = 2k_b \mathcal{D}$	drift velocity	$l_0 = \sqrt{8\mathcal{D}t}$	diffusion length
$I_{in} = \mathcal{D}k_{in}^2$	input current	$I_{out}(t) = -\frac{\mathcal{D}}{2}\partial_1^2 E(L, L; t)$	output current
$\eta_L(t) = I_{out}(t)/I_{in}$	current ratio	$\rho(x; t) = \frac{1}{2}(\partial_1 - \partial_2)E(x, x; t)$	local particle concentration
$I(x; t) = v\rho(x; t)$	local current	$\mathcal{N}_L = \int_0^L \rho(x; t) dx$	number of particles
$\rho_L(t) = L^{-1} \int_0^L \rho(x; t) dx$	averaged concentration	$\Lambda = \sqrt{k_b^2 - k_{in}^2}$	effective wavenumber
$t_L = L^2/(8\mathcal{D})$	characteristic time	$\epsilon = L^2/l_0^2 = t_L/t$	inverse time parameter

Appendix A.

Expression of the interval probability function Eq. (22) contains integrals independent of the initial conditions that can be performed exactly, except for the contribution

$$\int_0^\infty \int_0^\infty dx'_1 dx'_2 \left[K(x_2, x'_1)K(x_1, x'_2) - K(x_1, x'_1)K(x_2, x'_2) \right] \theta(x'_2 - x'_1) =: \mathcal{F}_k(x_1, x_2) - \mathcal{F}_k(x_2, x_1)$$

with function \mathcal{F}_k is given, after performing a first integration, by

$$\mathcal{F}_k(x_1, x_2) = \int_0^\infty \frac{dy}{4\sqrt{\pi\mathcal{D}t}} \left[\exp \left\{ -\frac{(x_2 - y - 2k\mathcal{D}t)^2}{4\mathcal{D}t} \right\} - e^{2kx_2} \exp \left\{ -\frac{(x_2 + y + 2k\mathcal{D}t)^2}{4\mathcal{D}t} \right\} \right] \times$$

$$\left[\operatorname{erfc} \left(\frac{-x_1 + y + 2k\mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) - e^{2kx_1} \operatorname{erfc} \left(\frac{x_1 + y + 2k\mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) \right]. \quad (\text{A.1})$$

This integral can be rewritten in a more compact form as

$$\begin{aligned} \mathcal{F}_k(x_1, x_2) &= -\frac{1}{4} \int_0^\infty dy \mathcal{G}_k(x_1, y) \partial_y \mathcal{G}_k(x_2, y), \\ \mathcal{G}_k(x, y) &:= \operatorname{erfc} \left(\frac{-x + y + 2k\mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right) - \exp(2kx) \operatorname{erfc} \left(\frac{x + y + 2k\mathcal{D}t}{2\sqrt{\mathcal{D}t}} \right). \end{aligned} \quad (\text{A.2})$$

After performing one integration by parts, we find that the contribution $\rho_1(x, k; t)$ to the density is given by

$$\begin{aligned} \rho_1(x, k; t) &= (\partial_{x_1} \mathcal{F}_k(x_1, x_2) - \partial_{x_1} \mathcal{F}_k(x_2, x_1))_{x_1=x_2=x} \\ &= -\frac{1}{2} \int_0^\infty dy \partial_x \mathcal{G}_k(x, y) \partial_y \mathcal{G}_k(x, y) - \frac{1}{4} \partial_x \mathcal{G}_k(x, 0) \mathcal{G}_k(x, 0) \end{aligned} \quad (\text{A.3})$$

The integral can be performed partially, leading to erf dependent functions in the expression of ρ_1 , Eq. (25).

Appendix B.

In this appendix, we propose to express functions $\Psi_s(x, y)$ and $\chi_s(x, y)$ using elliptic functions. In general, we will need to know the explicit expression in terms of elliptic function of the Gaussian series $G_{\alpha, \beta}^\pm(z)$ defined by

$$G_{\alpha, \beta}^\pm(z) := \sum_{n=-\infty}^{+\infty} (\pm 1)^n e^{-\alpha(z-n)^2 + 2i\beta n}, \quad \alpha > 0. \quad (\text{B.1})$$

In particular, these series are complex, with conjugation relation

$$\overline{G_{\alpha, \beta}^\pm(z)} = G_{\alpha, \beta}^\pm(-z). \quad (\text{B.2})$$

We can relate these Gaussian series with the periodic Jacobi elliptic functions θ_3 and θ_4 which are simply defined by the series expansions

$$\theta_3(z, q) = 1 + 2 \sum_{n=1}^{\infty} q^{n^2} \cos(2nz), \quad \theta_4(z, q) = 1 + 2 \sum_{n=1}^{\infty} (-1)^n q^{n^2} \cos(2nz) = \theta_3(z \pm \frac{\pi}{2}, q). \quad (\text{B.3})$$

The sum in Eq. (B.1) can be rearranged so that $G_{\alpha, \beta}^+(z) = e^{-\alpha z^2} \theta_3(i\alpha z - \beta, e^{-\alpha})$ and $G_{\alpha, \beta}^-(z) = e^{-\alpha z^2} \theta_4(i\alpha z - \beta, e^{-\alpha})$. In this case, we can rewrite Ψ_s as

$$\begin{aligned}
\Psi_s(x, y) &= \sqrt{\frac{2}{\pi l_0^2}} \left\{ G_{8L^2/l_0^2, 0}^- \left(\frac{x-y}{2L} \right) - G_{8L^2/l_0^2, 0}^- \left(\frac{x+y}{2L} \right) \right\} \\
&= \sqrt{\frac{2}{\pi l_0^2}} \left\{ e^{-\frac{2}{l_0^2}(x-y)^2} \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) - e^{-\frac{2}{l_0^2}(x+y)^2} \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x+y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) \right\}.
\end{aligned} \tag{B.4}$$

For $\chi_s(x, y)$, we obtain instead

$$\begin{aligned}
\chi_s(x, y) &= \sum_n \mathcal{W}_{l_0}(x-y-2nL) \varphi_n(y) + \mathcal{W}_{l_0}(x-y-L-2nL) \varphi_n(y+L) \\
&= \sqrt{\frac{2}{\pi l_0^2}} \frac{1}{\cos(k_{in}L)} \text{Re} \left\{ e^{ik_{in}(y-L)} G_{8L^2/l_0^2, k_{in}L}^+ \left(\frac{x-y}{2L} \right) - e^{ik_{in}(y-L)} G_{8L^2/l_0^2, 0}^- \left(\frac{x-y}{2L} \right) \right\} + (y \rightarrow y+L) \\
&= \sqrt{\frac{2}{\pi l_0^2}} \frac{e^{-\frac{2}{l_0^2}(x-y)^2}}{\cos(k_{in}L)} \text{Re} e^{ik_{in}(y-L)} \left\{ \theta_3 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L} - k_{in}L, e^{-\frac{8L^2}{l_0^2}} \right) \right. \\
&\quad \left. - \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) \right\} + (y \rightarrow y+L) \\
&= \sqrt{\frac{2}{\pi l_0^2}} \frac{e^{-\frac{2}{l_0^2}(x-y)^2}}{\cos(k_{in}L)} \left\{ \text{Re} \left[e^{ik_{in}(y-L)} \theta_3 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L} - k_{in}L, e^{-\frac{8L^2}{l_0^2}} \right) \right] \right. \\
&\quad \left. - \cos[k_{in}(y-L)] \theta_4 \left(\frac{4iL^2}{l_0^2} \frac{x-y}{L}, e^{-\frac{8L^2}{l_0^2}} \right) \right\} + (y \rightarrow y+L).
\end{aligned} \tag{B.5}$$

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